

- After a recap of generative chemistries and the DPO approach, we will discuss i.) the ILP formulation for autocatalysis, ii.) (sub-)graph isomorphism (Ullmann's algorithms) and iii.) graph canonicalization. Also, I'll introduce you to the strategy framework of `mød`.
  
- Mandatory Reading:
  - Main source of information: Chapter 4 of the PhD thesis by Jakob Lykke Andersen.
  
- Highly Recommended Reading if you are more interested:
  - Jakob L. Andersen, Daniel Merkle. *A Generic Framework for Engineering Graph Canonization Algorithms*. *Journal of Experimental Algorithms*, 2019 (in press). (This is the journal version of the proceedings paper of the Twentieth Workshop on Algorithm Engineering and Experiments (ALENEX, 2018))  
<https://epubs.siam.org/doi/abs/10.1137/1.9781611975055.13>
  - Source Code related to the article:
    - \* [https://github.com/jakobandersen/graph\\_canon](https://github.com/jakobandersen/graph_canon)
    - \* [https://github.com/jakobandersen/perm\\_group](https://github.com/jakobandersen/perm_group)
    - \* [https://github.com/jakobandersen/graph\\_canon\\_vis](https://github.com/jakobandersen/graph_canon_vis)
  - McKay, B.D. and Piperno, A., Practical Graph Isomorphism, II, *Journal of Symbolic Computation*, 60 (2014), pp.94-112.
  - S. G. Hartke and A. Radcliffe. *McKay's canonical graph labeling algorithm*. In *Communicating Mathematics*, volume 479 of *Contemporary Mathematics*, pages 99-111. American Mathematical Society, (2009). This article contains the example for the handwritten notes.